

Symmetries and time operators

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Abstract. All covariant time operators with normalized probability distribution are derived. Symmetry criteria are invoked to arrive at a unique expression for a given Hamiltonian. As an application, a well known result for the arrival time distribution of a free particle is generalized and extended. Interestingly, the resulting arrival time distribution operator is connected to a particular, positive, quantization of the classical current. For particles in a potential we also introduce and study the notion of conditional arrival-time distribution.

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1. Introduction

In spite of a famous footnote by Pauli [1] on the purported non-existence of a time operator in quantum mechanics, physically motivated questions relating to time occur quite naturally in the form of arrival times or of time durations. These become interesting when the extension of the wavefunction comes into play, and a quantum mechanical description by operators is not at all obvious. Also clock time operators have been investigated in the literature. For reviews of several aspects of these difficulties and of some more recent results see, e.g. [2, 3]. As quite recently stressed by us and Muñoz in [4], for a given system there is no single time operator. Indeed, there may be many, corresponding to different observables and measuring devices.

There are two main groups of physically relevant time operators. These are associated with time durations and time instants, respectively. An example of a duration is the dwell time of a particle in a region of space. The corresponding operator commutes with the Hamiltonian since the duration does not depend on a particular reference instant [5]. In the other group, the time observables are covariant in the sense that

when the preparation time is shifted they are shifted by the same amount, either forward (quantum clocks) [6] or backward (event times recorded with a stopwatch, e.g. time of arrival), and they are conjugate to the Hamiltonian.

The measurement of a clock time operator \hat{T} is supposed to yield, up to a constant, the parametric time. More precisely, \hat{T} should satisfy $\langle\psi_t|\hat{T}|\psi_t\rangle = t + \langle\psi_0|\hat{T}|\psi_0\rangle$. Time-of-arrival operators are mathematically similar to clock time operators, but the physics is different. Some of their properties are motivated by the behaviour of a classical particle, and in any case may be put at test experimentally. A free particle in one dimension must, during its motion, arrive at a given point with certainty, and it must also arrive in three dimensions at an infinitely extended plane. On a half-line, a free particle is reflected at the end point and may therefore arrive twice at another point. In this case it is reasonable to investigate *first* (or second) arrivals at a point [4]. The most difficult case is a particle interacting with an external potential [7, 8, 9, 10, 11, 12]. The particle can be deflected and, in one dimension, reflected so that it may, with a non-zero probability, never arrive at a particular position. In such a case it is then natural to ask for the probability distribution of first arrival at time t , given that the particle is arriving at all, i.e. to ask for the *conditional* first-arrival probability distribution, which is, by definition, normalized to 1. In [4] the most general form of covariant and normalized time observables was announced and a proof of a special case was indicated. The general proof of this result will be given in this paper. Reference [4] also gave applications to arrival times for a free particle on a half line and to Lyapunov operators in quantum mechanics. Based on physically motivated postulates pertaining to arrivals at a plane in three dimensions, [13] and [14] derived a time-of-arrival operator for a free particle in three dimensions coming in from one side of the plane. Among the postulates were invariance of the time operator under Galilei transformations, which leave invariant the plane in question, and minimal means-square deviation. This result will be generalized in the present paper and the underlying conditions will be weakened. In particular, Galilei invariance will not be needed.

The plan of the paper is as follows. In Section 2 we study covariant and normalized time observables and explicitly spell out their most general form, with the detailed proof referred to the Appendix. In Section 3 we analyze physical conditions, in particular symmetry conditions, under which time observables become unique, and discuss applications to clock-time operators. In Section 4 we give applications to time-of-arrival operators for free particles in one and three dimensions. In particular, the result of [13, 14] will be generalized. The restriction on the incoming direction will be lifted and the above Galilei invariance will be replaced by invariance under translations which leave the plane in question invariant. It will be shown that the resulting arrival time distribution and operator are related to a particular, positive, quantization of the classical current. Due to the backflow effect [15] the usual quantization in the form of the quantum mechanical probability does not have the necessary positivity properties. In Section 5 we study the notion of first arrivals in the presence of a potential and the associated probability distribution operator, which in general is not normalized to 1.

Normalizing by the total arrival probability for a given state one obtains the conditional arrival probability distribution which is normalized, but, by construction, is not bilinear in the wavefunction. Alternatively, to keep bilinearity we consider normalization by means of an operator and the resulting distribution operators. A one-dimensional example for a particle in a potential symmetric about the origin and arrivals at the origin is discussed. In the Appendix mathematical fine points such as regularity properties are discussed.

2. Clock time and time-of-arrival operators

Clock time operators can be associated with a quantum clock whose average measures the progressing parametric time. A good clock would also minimize the variance in order to estimate the time as accurately as possible with a finite number of measurements.

For a clock observable, let the probability of finding the measured time in the interval (∞, τ) for a state $|\psi\rangle$ be given by the expectation of an operator \hat{F}_τ , which plays the role of a cumulative probability operator, so that $\hat{F}_\infty = \mathbb{1}$. The derivative $d\langle\psi|\hat{F}_\tau|\psi\rangle/d\tau$ is the corresponding temporal probability distribution and it is normalized to 1. For a momentum measurement the analogous operator would be a projector, while here one just has $0 \leq \hat{F}_\tau \leq 1$ with selfadjoint \hat{F}_τ . The collection of \hat{F}_τ 's yields a positive operator-valued measure. We define the probability distribution operator $\hat{\Pi}_\tau$ and the time operator \hat{T} by

$$\begin{aligned}\hat{\Pi}_\tau &\equiv \frac{d}{d\tau} \hat{F}_\tau, \\ \hat{T} &\equiv \int d\tau \tau \hat{\Pi}_\tau.\end{aligned}\tag{1}$$

For details on the derivative see the Appendix. The mean value of observed time can be written as

$$\langle\psi| \int d\tau \tau \hat{\Pi}_\tau |\psi\rangle \equiv \langle\psi|\hat{T}|\psi\rangle.\tag{2}$$

The second moment, if it exists, is given by $\langle\psi| \int d\tau \tau^2 \hat{\Pi}_\tau |\psi\rangle$ and similarly for higher moments.

Covariance of a clock time operator with respect to ordinary (parametric) time means that the probabilities of finding the measured time in the interval $(-\infty, \tau)$ for state $|\psi_0\rangle$ and in $(-\infty, \tau + t)$ for $|\psi_t\rangle$ coincide. This implies

$$\hat{F}_\tau = e^{-i\hat{H}\tau/\hbar} \hat{F}_0 e^{i\hat{H}\tau/\hbar}.\tag{3}$$

From this one obtains by differentiation (see the Appendix for details)

$$\hat{\Pi}_0 = \frac{-i}{\hbar} [\hat{H}, \hat{F}_0],\tag{4}$$

$$\hat{\Pi}_\tau = e^{-i\hat{H}\tau/\hbar} \hat{\Pi}_0 e^{i\hat{H}\tau/\hbar}.\tag{5}$$

Note that $\hat{\Pi}_0$ and $\hat{\Pi}_\tau$ are in general not operators on the Hilbert space but only bilinear forms evaluated between normalizable vectors from the domain of \hat{H} . Since $\langle\psi|\hat{F}_\tau|\psi\rangle$

is non-decreasing, $\hat{\Pi}_\tau$ is a positive bilinear form. An expression like $\langle E | \hat{\Pi}_0 | E' \rangle$ has to be understood as a distribution. Since the diagonal $E = E'$ has measure 0 it is no contradiction that (4) formally gives 0 on the diagonal while explicit examples may give a non-zero value [4]. By a change of variable in (1) one obtains

$$e^{i\hat{H}t/\hbar} \hat{T} e^{-i\hat{H}t/\hbar} = \hat{T} + t. \quad (6)$$

Furthermore, \hat{H} and \hat{T} satisfy the canonical commutation relations as bilinear forms on a suitable domain.

A superscript A denotes quantities for (first) arrival times at a given location. In contrast to clock times, if the particle's state is shifted in time by t_0 , it should arrive a time t_0 earlier, and the temporal probability distribution should be shifted by t_0 to earlier times. Thus the analog of the cumulative probability operator in (3) and the probability density operator must now satisfy

$$\hat{F}_t^A = e^{i\hat{H}t/\hbar} \hat{F}_0^A e^{-i\hat{H}t/\hbar}, \quad (7)$$

$$\hat{\Pi}_0^A = \frac{i}{\hbar} [\hat{H}, \hat{F}_0^A], \quad (8)$$

$$\hat{\Pi}_t^A = e^{i\hat{H}t/\hbar} \hat{\Pi}_0^A e^{-i\hat{H}t/\hbar}. \quad (9)$$

Again, $\hat{\Pi}_\tau^A$ is a positive bilinear form.

In case of a particle in a potential, it may happen that for a given state the particle arrives at the location with a total probability less than 1. This means that the integral of $\hat{\Pi}_t^A$ is not unity. For the average arrival time one can then not use the left-hand side of the analog of (2) but rather

$$\langle \psi | \int d\tau \tau \hat{\Pi}_\tau | \psi \rangle / \langle \psi | \hat{N} | \psi \rangle, \quad (10)$$

where $\hat{N} \equiv \int d\tau \hat{\Pi}_\tau = \hat{F}_\infty$. However, if the total arrival probability is always 1, one can define an arrival time operator by

$$\hat{T}^A = \int d\tau \tau \hat{\Pi}_\tau \quad (11)$$

$$= \int dt t e^{i\hat{H}t/\hbar} \hat{\Pi}_0^A e^{-i\hat{H}t/\hbar}. \quad (12)$$

As seen by a change of integration variable, an arrival time operator behaves as the negative of a clock time operator whose probability distribution operator is given by $\hat{\Pi}_\tau = \hat{\Pi}_{-\tau}^A$, with a cumulative probability operator $\hat{F}_\tau = \mathbb{1} - \hat{F}_{-\tau}^A$.

We now prove the following general result for covariant clock operators and arrival time operators with normalized distributions. This was already announced in [4] without proof. In Appendix A.1 and Appendix A.2 we present rigorous mathematical details.

Let \hat{H} be a Hamiltonian with purely continuous eigenvalues and eigenvectors $|E, \alpha\rangle$, where the degeneracy index can be assumed to be a discrete number. Their normalization is taken as

$$\langle E, \alpha | E', \alpha' \rangle = \delta_{\alpha\alpha'} \delta(E - E'). \quad (13)$$

For simplicity we assume the same degeneracy for each E . We consider any covariant clock time operator which has a probability distribution normalized to 1 and whose second moment exists for a dense set of vectors. Then for $t = 0$ the probability distribution $\hat{\Pi}_0$ is given by

$$\begin{aligned}\hat{\Pi}_0 &= \frac{1}{2\pi\hbar} \sum_i |b_i\rangle\langle b_i| \\ &= \frac{1}{2\pi\hbar} \sum_i \int dE dE' \sum_{\alpha\alpha'} b_i(E, \alpha) |E, \alpha\rangle\langle E', \alpha'| \overline{b_i(E', \alpha')},\end{aligned}\quad (14)$$

where $b_i(E, \alpha) \equiv \langle E, \alpha | b_i \rangle$ are any functions satisfying the two conditions

$$\sum_i b_i(E, \alpha) \overline{b_i(E, \alpha')} = \delta_{\alpha\alpha'}, \quad (15)$$

$$\sum_i |\partial_E b_i(E, \alpha)|^2 \text{ integrable over finite intervals.} \quad (16)$$

The same results hold for $\hat{\Pi}_0^A$ of normalized arrival time distributions. The complete distributions $\hat{\Pi}_t$ and $\hat{\Pi}_t^A$ and the associated time operators are then given by (1) - (5) and (7) - (11), respectively.

For a state $|\psi\rangle$, with $\psi(E, \alpha) \equiv \langle E, \alpha | \psi \rangle$, one has

$$\begin{aligned}\langle \psi | \hat{T} | \psi \rangle &= \int dE \sum_{\alpha} \overline{\psi(E, \alpha)} i\hbar \partial_E \psi(E, \alpha) \\ &+ \int dE \sum_{\alpha\alpha'} \overline{\psi(E, \alpha)} \psi(E, \alpha') \sum_i b_i(E, \alpha) i\hbar \partial_E \overline{b_i(E, \alpha')}\end{aligned}\quad (17)$$

$$\text{second moment} = \hbar^2 \int dE \left| \partial_E \sum_{\alpha} \overline{b_i(E, \alpha)} \psi(E, \alpha) \right|^2. \quad (18)$$

A mathematically detailed proof will be given in Appendix A.1 and Appendix A.2. For simplicity we indicate here a formal proof for the case that the (continuous) eigenvalues of \hat{H} are non-degenerate. We start by constructing the functions b_i . For a given $\hat{\Pi}_0$, one can choose a maximal set $\{|g_i\rangle\}$ of vectors satisfying

$$\langle g_i | \hat{\Pi}_0 | g_j \rangle = \delta_{ij}. \quad (19)$$

Such a maximal set is easily constructed by the standard Schmidt orthogonalization procedure. Then a possible set of $|b_i\rangle$'s is given by

$$|b_i\rangle = \sqrt{2\pi\hbar} \hat{\Pi}_0 |g_i\rangle. \quad (20)$$

Indeed, from (20) one has

$$\begin{aligned}\frac{1}{2\pi\hbar} \sum_i \langle g_{\alpha} | b_i \rangle \langle b_i | g_{\beta} \rangle &= \sum_i \langle g_{\alpha} | \hat{\Pi}_0 | g_i \rangle \langle g_i | \hat{\Pi}_0 | g_{\beta} \rangle \\ &= \sum_i \delta_{\alpha i} \delta_{\beta i} = \delta_{\alpha\beta}.\end{aligned}\quad (21)$$

Equation (19) then implies

$$\hat{\Pi}_0 = \frac{1}{2\pi\hbar} \sum_i |b_i\rangle\langle b_i|, \quad (22)$$

which is (14). It should be noted that the $|b_i\rangle$'s in the decomposition of $\hat{\Pi}_0$ in (14) are not unique.

The $|b_i\rangle$'s need not be normalizable and the $b_i(E)$'s could in principle be distributions. That the $b_i(E)$'s are in fact functions will be shown in Appendix A.1. They have to satisfy certain properties in order that the total probability is 1 and that the second moment is finite. Indeed, for given normalized state $|\psi\rangle$, the total temporal probability is, with $\psi(E) \equiv \langle E|\psi\rangle$,

$$\begin{aligned}
& \int_{-\infty}^{+\infty} \frac{dt}{2\pi} \langle \psi | e^{-i\hat{H}t/\hbar} \hat{\Pi}_0 e^{i\hat{H}t/\hbar} | \psi \rangle \\
&= \sum_i \int \frac{dt}{2\pi\hbar} \int dE dE' e^{-i(E-E')t/\hbar} \overline{\psi(E)} b_i(E) \overline{b_i(E')} \psi(E') \\
&= \sum_i \int dE dE' \delta(E-E') \overline{\psi(E)} b_i(E) \overline{b_i(E')} \psi(E') \\
&= \sum_i \int dE \overline{\psi(E)} \sum_i b_i(E) \overline{b_i(E)} \psi(E) \stackrel{!}{=} 1 .
\end{aligned} \tag{23}$$

Since $|\psi\rangle$ is arbitrary this implies

$$\sum_i b_i(E) \overline{b_i(E)} = 1 . \tag{24}$$

The formal use of the δ function will be justified in Appendix A.1. In a similar way one obtains

$$\begin{aligned}
\langle \psi | \hat{T} | \psi \rangle &= \int dE \bar{\psi}(E) i\hbar \psi'(E) \\
&+ \int dE |\psi(E)|^2 \sum_i b_i(E) i\hbar \overline{b'_i(E)} .
\end{aligned} \tag{25}$$

Note that $\sum_i b_i \bar{b}'_i$ is purely imaginary, from (24), and thus vanishes if b_i is real. The second moment is

$$\begin{aligned}
& \int \frac{dt}{2\pi} t^2 \langle \psi | e^{-i\hat{H}t/\hbar} \hat{\Pi}_0 e^{i\hat{H}t/\hbar} | \psi \rangle \\
&= \hbar \sum_i \int \frac{dt}{2\pi} \int dE dE' \partial_E \partial_{E'} e^{-i(E-E')t/\hbar} \overline{\psi(E)} b_i(E) \overline{b_i(E')} \psi(E') \\
&= \hbar^2 \sum_i \int dE \partial_E \left(\overline{\psi(E)} b_i(E) \right) \partial_E \left(\overline{b_i(E)} \psi(E) \right) \\
&= \hbar^2 \int dE \{ |\psi'(E)|^2 + \sum_i |b'_i(E)|^2 |\psi(E)|^2 \\
&\quad + 2 \operatorname{Re} \sum_i \overline{b_i(E)} b'_i(E) \overline{\psi(E)} \psi'(E) \}
\end{aligned} \tag{26}$$

by (24). This is finite if the contribution from the first and second term are finite, and for the latter to hold for all infinitely differentiable functions $\psi(E)$ with compact support one must have that $\sum_i |b'_i(E)|^2$ is integrable over any finite interval. Again,

differentiability of the b_i 's will be shown in the Appendix, as well as the proof in the case that \hat{H} has degenerate eigenvalues.

Conversely, it is easily checked that any functions $b_i(E, \alpha)$ which satisfy (15) and (16) give rise to a covariant time operator with normalized probability distribution and second moment for a dense set of vectors.

3. Degenerate energy eigenstates: unique clock time operators from symmetry and minimal variance

Clock time operators have a normalized probability distribution, and this will be assumed in the following. To reduce the multitude of covariant clock time operators we may require that the variance ΔT , or mean-square deviation ΔT^2 , is minimal for all states for which the second moment exists. Physically this means that no other time observable can be measured more precisely. However, requiring minimal variance by itself does not make \hat{T} unique, not even in the case of non-degenerate spectrum of \hat{H} , as was shown in Ref. [4]. But if in addition one restricts the set of functions b_i by symmetry requirements, uniqueness may then follow from minimality of ΔT , as will be illustrated now.

We denote the anti-unitary time reversal operator by $\hat{\Theta}$. In the \mathbf{x} space representation one has $(\hat{\Theta}\psi)(\mathbf{x}) = \overline{\psi(\mathbf{x})}$. If the Hamiltonian is time reversal invariant, we may demand

$$\hat{\Theta} \hat{T} \hat{\Theta} = -\hat{T} \quad (27)$$

and similarly for the probability distribution. By (3) this implies

$$\hat{\Theta} \hat{\Pi}_0 \hat{\Theta} = \hat{\Pi}_0. \quad (28)$$

In [4] it was shown for the non-degenerate eigenvalue case that time reversal invariance of the Hamiltonian \hat{H} and minimal ΔT together imply that \hat{T} and $\hat{\Pi}_t$ are unique and given by

$$\begin{aligned} \hat{\Pi}_t &= \frac{1}{2\pi\hbar} \int dE dE' e^{-i(E-E')t/\hbar} |E_\Theta\rangle \langle E'_\Theta|, \\ \hat{T} &= \int dt t \hat{\Pi}_t, \end{aligned} \quad (29)$$

with time reversal invariant $|E_\Theta\rangle$.

If the Hamiltonian has degenerate continuous eigenvalues this is no longer true and one needs additional conditions to obtain uniqueness, as discussed now.

Example 1: In one dimension we consider

$$\hat{H} = \hat{P}^2/2m + V(|\hat{X}|) \quad (30)$$

and assume a purely continuous spectrum. \hat{H} is invariant under space reflection, denoted by $\hat{\sigma}$, and under time reversal $\hat{\Theta}$. We assume \hat{T} and its probability distribution to have analogous properties. For $\hat{\Pi}_0$ this implies

$$\hat{\sigma} \hat{\Pi}_0 \hat{\sigma} = \hat{\Theta} \hat{\Pi}_0 \hat{\Theta} = \hat{\Theta} \hat{\sigma} \hat{\Pi}_0 \hat{\sigma} \hat{\Theta} = \hat{\Pi}_0. \quad (31)$$

Then, under the assumption of normalizability, the time operator becomes unique, as shown now. As eigenstates of \hat{H} we choose real and either symmetric or antisymmetric wavefunctions, denoted by $|E, \pm\rangle$ and normalized as $\delta(E - E')$. Then $\hat{\Theta}|E, \pm\rangle = |E, \pm\rangle$ and $\hat{\sigma}|E, \pm\rangle = \pm|E, \pm\rangle$. Decomposing the functions $b_{i\alpha}$ in (14) for $\hat{\Pi}_0$ into real and imaginary parts one finds from $\hat{\Pi}_0 = \frac{1}{2}(\hat{\Pi}_0 + \hat{\Theta}\hat{\Pi}_0\hat{\Theta})$ that (14) can be written with real functions when one uses $|E, +\rangle$ and $|E, -\rangle$ as basis. Writing again $\hat{\Pi}_0 = \frac{1}{2}(\hat{\Pi}_0 + \hat{\sigma}\hat{\Pi}_0\hat{\sigma})$ one sees that the mixed $\alpha\alpha'$ terms cancel so that one can write $\hat{\Pi}_0$ in the form

$$\hat{\Pi}_0 = \frac{1}{2\pi\hbar} \sum_i \sum_{\alpha=\pm} \int dE dE' b_{i\alpha}(E) |E, \alpha\rangle \langle E', \alpha| b_{i\alpha}(E') \quad (32)$$

with real functions $b_{i\alpha}$. Note that (32) has no mixed $\alpha\alpha'$ terms and is in this sense diagonal. The normalization condition (15) is replaced by

$$\sum_i b_{i\alpha}(E)^2 = 1 \quad , \quad \alpha = \pm . \quad (33)$$

Diagonality in α and reality of the functions $b_{i\alpha}$ will be crucial for determining $b_{i\alpha}$ explicitly. In fact, expanding the right-hand side of (18) for the second moment, the term

$$\sum_{i\alpha\alpha'} \int dE b'_i(E\alpha) \overline{b_i(E, \alpha')} \overline{\psi(E, \alpha)} \psi'(E, \alpha') + \text{c.c.} \quad (34)$$

is replaced by

$$\sum_{i\alpha} \int dE b'_{i\alpha}(E) b_{i\alpha}(E) \left\{ \overline{\psi(E, \alpha)} \psi'(E, \alpha) + \text{c.c.} \right\} \quad (35)$$

and similarly for an analogous term in $\langle \psi | \hat{T} | \psi \rangle$. Now, one has

$$\sum_i b'_{i\alpha}(E) b_{i\alpha}(E) = \frac{1}{2} \partial_E \sum_i b_{i\alpha}(E)^2 = 0 \quad (36)$$

by (33). Therefore the only $b_{i\alpha}$ dependent term in ΔT^2 is

$$\sum_{i\alpha} \int dE |b'_{i\alpha}(E)|^2 |\psi(E, \alpha)|^2. \quad (37)$$

This becomes minimal if and only if $b'_{i\alpha} \equiv 0$, i.e.

$$b_{i\alpha}(E) \equiv c_{i\alpha}, \quad (38)$$

with the real constant $c_{i\alpha}$ satisfying, by (33),

$$\sum_i (c_{i\alpha})^2 = 1 \quad , \quad \alpha = \pm . \quad (39)$$

Inserting this into (32) gives finally

$$\hat{\Pi}_0 = \frac{1}{2\pi\hbar} \int dE dE' \{ |E, +\rangle \langle E', +| + |E, -\rangle \langle E', -| \} . \quad (40)$$

From (3) and (1) one now obtains the corresponding operators $\hat{\Pi}_t$ and \hat{T} . Thus, in this one-dimensional example, covariance under time reversal and reflection plus minimality

of ΔT lead to a unique clock time operator and a unique associated temporal probability distribution.

Interestingly, when the potential V in (30) allows the application of scattering theory, $\hat{\Pi}_0$ in (40) can be re-expressed in terms of the Møller operators $\hat{\Omega}_\pm$ and complex reflection and transmission coefficients, $T(k)$ and $R(k)$. We denote by $|k\rangle$ momentum eigenstates. Reflection invariance gives $\hat{\sigma}\hat{\Omega}_\pm\hat{\sigma} = \hat{\Omega}_\pm$ and $R(-k) = R(k)$, $T(-k) = T(k)$. The interpolation property $\hat{H}\hat{\Omega}_\pm = \hat{\Omega}_\pm\hat{H}_0$ shows that the two vectors

$$\begin{aligned} &(\hat{\Omega}_+ + \hat{\Omega}_-)(|k\rangle + |-k\rangle)/\sqrt{2} \\ &i(\hat{\Omega}_+ - \hat{\Omega}_-)(|k\rangle - |-k\rangle)/\sqrt{2} \end{aligned} \quad (41)$$

are eigenvectors of \hat{H} which are symmetric and antisymmetric, respectively, and invariant under $\hat{\sigma}\hat{\Theta}$ since $\hat{\Theta}\hat{\Omega}_\pm\hat{\Theta} = \hat{\Omega}_\mp$. Hence the vectors in (41) are real multiples of $|E, \pm\rangle$. To determine the respective multiple we use the identities

$$\hat{\Omega}_+ + \hat{\Omega}_- = \hat{\Omega}_-(\hat{S} + 1) = \hat{\Omega}_+(1 + \hat{S}^\dagger), \quad (42)$$

$$\hat{S}|k\rangle = T(k)|k\rangle + R(k)|-k\rangle. \quad (43)$$

Thus

$$\hat{S}(|k\rangle \pm |-k\rangle) = (T(k) \pm R(k))(|k\rangle \pm |-k\rangle). \quad (44)$$

This implies that here $T(k) \pm R(k)$ are pure phases. With (42) the two vectors in (41) become

$$\begin{aligned} &(1 + \overline{T(k)} + \overline{R(k)})\hat{\Omega}_+(|k\rangle + |-k\rangle)/\sqrt{2}, \\ &i(1 + \overline{T(k)} - \overline{R(k)})\hat{\Omega}_+(|k\rangle - |-k\rangle)/\sqrt{2}. \end{aligned} \quad (45)$$

Hence, from normalization one finds

$$|E, \pm\rangle = \frac{i^{(1\mp 1)/2} \sqrt{m/\hbar^2 k}}{|1 + T(k) + R(k)|} (\hat{\Omega}_+ + \hat{\Omega}_-)(|k\rangle \pm |-k\rangle)/\sqrt{2}. \quad (46)$$

Using (44) this can be re-expressed by T, R , and $\hat{\Omega}_+$ as

$$|E, \pm\rangle = i^{(1\mp 1)/2} \sqrt{\frac{m}{\hbar^2 k}} \frac{1 + \bar{T} \pm \bar{R}}{|1 + T \pm R|} \hat{\Omega}_+(|k\rangle \pm |-k\rangle)/\sqrt{2}. \quad (47)$$

Inserting this into (40) and introducing k as integration variable, $E/\hbar = \hbar k^2/2m$, one obtains an expression for $\hat{\Pi}_0$ with coherences between $|k\rangle$ and $|-k\rangle$. For a free particle in one dimension ($T = 1, R = 0, \hat{\Omega}_+ = \mathbb{1}$) one obtains

$$\hat{\Pi}_0^{(V=0)} = \frac{1}{2\pi m} \int_0^\infty dk \int_0^\infty dk' \sqrt{kk'} \{|k\rangle\langle k'| + |-k\rangle\langle -k'|\} \quad (48)$$

so that in the free case there are no coherences between positive and negative momenta.

Example 2: We consider the three-dimensional case of the Hamiltonian

$$\hat{H} = \frac{\hat{\mathbf{P}}^2}{2m} + V(\hat{r}) \quad (49)$$

and assume a purely continuous spectrum. \hat{H} is invariant under rotations, reflection $\hat{\sigma}_1$ at the $x_2 - x_3$ plane, i.e. $\phi \rightarrow \pi - \phi$ in spherical coordinates, and under time reversal. In the following we assume only invariance of \hat{T} and its probability distribution operator under rotations and covariance under the combined action $\hat{\sigma}_1 \hat{\Theta}$; this means the invariance of $\hat{\Pi}_0$ under these operations. Again this implies the existence of a unique time operator and its probability distribution, as shown now.

The eigenfunctions of \hat{H} can be chosen in the form $f_{El}(r)Y_{lm}(\vartheta, \phi)$, f_{El} real. We denote these states by $|Elm\rangle$, with the normalization

$$\langle Elm|E'l'm'\rangle = \delta(E - E')\delta_{ll'}\delta_{mm'} . \quad (50)$$

The action of $\hat{\sigma}_1 \hat{\Theta}$ is given by

$$\hat{\sigma}_1 \hat{\Theta}|Elm\rangle = (-1)^m |Elm\rangle . \quad (51)$$

Invariance under rotations and under $\hat{\sigma}_1 \hat{\Theta}$ implies that $\hat{\Pi}_0$ can be written in the form

$$\hat{\Pi}_0 = \frac{1}{2\pi\hbar} \sum_i \int dE dE' \sum_{lm} b_{ilm}(E) |Elm\rangle \langle E'lm| b_{ilm}(E'), \quad (52)$$

with real functions b_{ilm} . In principle, the allowed set of l and m in the sum might depend on E , E' . However, if scattering theory can be applied this is not so, as seen further below. Note the diagonality in l, m . The condition for the functions b_{ilm} , arising from the normalization of the probability, now reads

$$\sum_i (b_{ilm}(E))^2 = 1 \quad \text{for each } l, m . \quad (53)$$

Equations (34)-(37) remain the same, only with α replaced by lm , and therefore minimality of ΔT implies

$$\hat{\Pi}_0 = \frac{1}{2\pi\hbar} \sum_i \sum_{lm} \int dE dE' |Elm\rangle \langle E'lm| , \quad (54)$$

where $\langle \mathbf{x}|Elm\rangle = f_{El}(r)Y_{lm}(\vartheta, \phi)$, with f_{El} real. Thus also in this example the time operator is unique and there are no coherences between different lm values.

Using scattering theory, (54) can again be expressed by the Møller operators $\hat{\Omega}_\pm$ and partial waves shifts, δ_l . We write $|Elm\rangle_0$ when $V \equiv 0$. Then

$$\langle \mathbf{x}|Elm\rangle_0 = \sqrt{\frac{2}{\pi}} \sqrt{\frac{m}{\hbar^2 k}} j_l(kr) Y_{lm}(\vartheta, \Phi) \quad (55)$$

and, from rotation symmetry,

$$\hat{S} |Elm\rangle_0 = e^{2i\delta_l} |Elm\rangle_0 . \quad (56)$$

$\hat{\Omega}_\pm$ commutes with rotations and $\hat{\sigma}$, and again $\hat{\Theta} \hat{\Omega}_\pm \hat{\Theta} = \hat{\Omega}_\mp$. From $\hat{H} \hat{\Omega}_\pm = \hat{\Omega}_\pm \hat{H}_0$ it follows that $(\hat{\Omega}_+ + \hat{\Omega}_-)|Elm\rangle_0$ is an eigenstate of $\hat{H}, \hat{L}^2, \hat{L}_3$, and also of $\hat{\sigma}_1 \hat{\Theta}$ with eigenvalue $(-1)^m$. Therefore it is a real multiple of $|Elm\rangle$. To calculate this multiple we use (42) and obtain

$$(\hat{\Omega}_+ + \hat{\Omega}_-)|Elm\rangle_0 = (1 + e^{\mp 2i\delta_l}) \hat{\Omega}_\pm |Elm\rangle_0 . \quad (57)$$

Taking scalar products one obtains, from the unitarity of $\hat{\Omega}_\pm$,

$$|Elm\rangle = \frac{1}{|1 + e^{2i\delta_l}|} (\hat{\Omega}_+ + \hat{\Omega}_-) |Elm\rangle_0 \quad (58)$$

and, from (57),

$$|Elm\rangle = \frac{1 + e^{\mp 2i\delta_l}}{|1 + e^{2i\delta_l}|} \hat{\Omega}_\pm |Elm\rangle_0. \quad (59)$$

Inserting this into (54) for $\hat{\Pi}_0$, using k as integration variable, where $E/\hbar = \hbar k^2/2m$, and the states

$$|klm\rangle_0 \equiv \hbar\sqrt{k/m} |Elm\rangle_0, \quad (60)$$

which are normalized to $\delta(k - k')\delta_{ll'}\delta_{mm'}$, then

$$\begin{aligned} \hat{\Pi}_0 = \hat{\Omega}_+ \frac{\hbar}{2\pi m} \sum_{lm} \int_0^\infty dk \int_0^\infty dk' \\ \sqrt{kk'} \frac{1 + e^{-2i\delta_l(k)}}{|1 + e^{2i\delta_l(k)}|} \frac{1 + e^{2i\delta_l(k')}}{|1 + e^{2i\delta_l(k')}|} |klm\rangle_{00} \langle k'lm| \hat{\Omega}_+^\dagger. \end{aligned} \quad (61)$$

The free particle case results if one puts $\Omega_+ = \mathbb{1}$ and $\delta_l = 0$.

4. Application to arrival times

Kijowski [13] considered, in three dimensions, a free particle of mass m coming in from $x_1 = -\infty$ and determined the distribution of times of arrival at a plane perpendicular to the x_1 axis, e. g. at $x_1 = 0$, by using physically motivated postulates. These were: covariance, normalization, invariance under all *Galilei* transformations which leave the plane $x_1 = 0$ invariant, invariance under the combined action of time reversal and space reflection $\sigma: \mathbf{x} \rightarrow -\mathbf{x}$, and minimal variance. His result, denoted here by $\hat{\Pi}_t^{Kij}$, for the probability distribution of particles with only positive momenta in the x_1 direction and for arrivals at the plane $x_1 = 0$, can be written as

$$\begin{aligned} \hat{\Pi}_t^{Kij} = \frac{\hbar}{2\pi m} \int_{-\infty}^\infty dk_2 dk_3 \int_0^\infty dk_1 \int_0^\infty dk'_1 \\ e^{i\hbar(k_1^2 - k'^1_2)t/2m} \sqrt{k_1 k'_1} |k_1, k_2, k_3\rangle \langle k'_1, k_2, k_3|. \end{aligned} \quad (62)$$

In the following, the methods of the previous sections will be used to generalize this result in two ways. First, invariance under Galilei transformations can be replaced by a weaker condition, and second, the restriction to particles coming in from one side can be lifted. We assume covariance, invariance under *translations* which leave the plane $x_1 = 0$ invariant, invariance under the space reflection $\sigma: \mathbf{x} \rightarrow -\mathbf{x}$, time reversal covariance, and minimal variance. These symmetry assumptions are taken over from the classical case. Indeed, if one has an ensemble of free classical particles and reflects each particle trajectory by σ , then the resulting reflected ensemble has the same distributions for arrivals at the plane $x_1 = 0$ as the original ensemble. In addition, one can go over to the time reversed trajectories, defined by $x_\theta(t) = x(-t)$. Then, if a particle arrives

at the plane at time t' , the corresponding particle on the time reversed trajectory will arrive there at time $-t'$. This implies that for the time reversed ensemble the arrival time distribution is obtained from the original one by replacing t by $-t$. Note that the arrival location, i.e. the plane $x_1 = 0$, is singled out here by the required reflection invariance under σ .

Under the above assumptions it will now be shown that Π_{ft}^A , the operator for the probability distribution of times of arrivals at the plane x_1 , is given by

$$\begin{aligned}\hat{\Pi}_{f0}^A &= \theta(\hat{v}_1) |\hat{v}_1|^{1/2} \delta(\hat{x}_1) |\hat{v}_1|^{1/2} \theta(\hat{v}_1) \\ &\quad + \theta(-\hat{v}_1) |\hat{v}_1|^{1/2} \delta(\hat{x}_1) |\hat{v}_1|^{1/2} \theta(-\hat{v}_1), \\ \hat{\Pi}_{ft}^A &= \exp\{i\hat{H}_0 t/\hbar\} \hat{\Pi}_{f0}^A \exp\{-i\hat{H}_0 t/\hbar\},\end{aligned}\tag{63}$$

where \hat{v}_1 and \hat{x}_1 are components of the velocity and position operator and $\theta(x)$ is the usual step function ($\theta(x) = 0$ for $x < 0$ and $\theta(x) = 1$ for $x > 0$). Note that classically the first term on the right-hand side corresponds to $\theta(v_1) v_1 \delta(x_1)$ which classically gives the number of particles crossing the plane x_1 per second from the left. Similarly for the second term, and their sum corresponds to $|v_1| \delta(x_1)$. Thus in this case the arrival time distribution operator can be regarded as a particular – positive – quantization of the classical current. The usual quantum mechanical probability current is not necessarily positive, not even for states with only positive momenta in the x_1 direction [15].

Inserting in (63) two complete sets of momentum eigenstates and using

$$\langle \mathbf{k} | \delta(\hat{x}_1) | \mathbf{k}' \rangle = \frac{1}{2\pi} \delta(k_2 - k'_2) \delta(k_3 - k'_3),\tag{64}$$

$\hat{\Pi}_{ft}^A$ can be written as

$$\begin{aligned}\hat{\Pi}_{ft}^A &= \frac{\hbar}{2\pi m} \int_{-\infty}^{\infty} dk_2 dk_3 \int_0^{\infty} dk_1 \int_0^{\infty} dk'_1 e^{i\hbar(k_1^2 - k'^2)t/2m} \\ &\quad \sqrt{k_1 k'_1} \{ |k_1, k_2, k_3\rangle \langle k'_1 k_2 k_3| + | -k_1, k_2, k_3\rangle \langle -k'_1, k_2, k_3| \}.\end{aligned}\tag{65}$$

For states with $k_1 > 0$ this reduces to (62). Note the absence of coherences between positive and negative k_1 values in the above expression. For dimensions d other than three an analogous result holds. For $d = 1$ it becomes, under a change $t \rightarrow -t$, identical to the clock time expression in (48).

To show (65) we introduce the notation

$$\begin{aligned}|\mathbf{k}, +\rangle &= (|k_1, k_2, k_3\rangle + | -k_1, k_2, k_3\rangle)/\sqrt{2}, \\ |\mathbf{k}, -\rangle &= i(|k_1, k_2, k_3\rangle - | -k_1, k_2, k_3\rangle)/\sqrt{2},\end{aligned}\tag{66}$$

which is a δ -normalized basis and invariant under $\hat{\sigma}\hat{\Theta}$ since $\hat{\sigma}\hat{\Theta}|\mathbf{k}\rangle = |\mathbf{k}\rangle$. The latter also implies that $\langle \mathbf{k} | \hat{\Pi}_{f0}^A | \mathbf{k}' \rangle$ must be real. One now has

$$\begin{aligned}\langle \mathbf{k}, + | \hat{\Pi}_{f0}^A | \mathbf{k}', + \rangle &= \langle \mathbf{k}, - | \hat{\Pi}_{f0}^A | \mathbf{k}', - \rangle = \langle \mathbf{k} | \hat{\Pi}_{f0}^A | \mathbf{k}' \rangle, \\ \langle \mathbf{k}, + | \hat{\Pi}_{f0}^A | \mathbf{k}', - \rangle &= 0.\end{aligned}\tag{67}$$

Translation invariance in the $x_1 = 0$ plane gives the general form

$$\langle \mathbf{k}, + | \hat{\Pi}_{f0}^A | \mathbf{k}', + \rangle = \delta(k_2 - k'_2) \delta(k_3 - k'_3) M(k_1, k_2, k_3, k'_1),\tag{68}$$

where, for fixed k_2 and k_3 , $M(\cdot, k_2, k_3, \cdot)$ is a positive definite kernel and one can write, with real functions $b_i(k_1; k_2, k_3)$,

$$M(k_1, k_2, k_3, k'_1) = \frac{\hbar}{2\pi m} \sum_i b_i(k_1; k_2, k_3) b_i(k'_1; k_2, k_3) \quad (69)$$

(cf. Appendix A.3 for more mathematical details). From this and (67) we obtain, with $|\mathbf{k}', \pm\rangle \equiv |k'_1 k_2, k_3, \pm\rangle$,

$$\begin{aligned} \hat{\Pi}_{f0}^A &= \frac{\hbar}{2\pi m} \sum_i \int_{-\infty}^{\infty} dk_2 \int_{-\infty}^{\infty} dk_3 \int_0^{\infty} dk_1 \int_0^{\infty} dk'_1 \\ &\quad b_i(k_1; k_2, k_3) \left\{ |\mathbf{k}, +\rangle \langle \mathbf{k}', +| + |\mathbf{k}, -\rangle \langle \mathbf{k}', -| \right\} b_i(k'_1; k_2, k_3). \end{aligned} \quad (70)$$

Note again the diagonality, this time in k_2 and k_3 . Since $\hat{\Pi}_{f0}^A$ commutes with translations and hence with the momentum operators \hat{P}_2 and \hat{P}_3 , the normalization condition for the probability distribution

$$\frac{1}{2\pi} \langle \psi | e^{i\hat{H}t/\hbar} \hat{\Pi}_{f0}^A e^{-i\hat{H}t/\hbar} | \psi \rangle \quad (71)$$

for states with $\langle \mathbf{k} | \psi \rangle$ vanishing at $k_1 = 0$, gives the condition

$$\begin{aligned} &\frac{\hbar}{m} \sum_i \int dk_1 dk_3 \int_0^{\infty} dk_1 dk'_1 \delta\left(\frac{\hbar}{2m}(k_1^2 - k'^2_1)\right) \\ &\quad \times b_i(k_1; k_2, k_3) b_i(k'_1; k_2, k_3) \left\{ \overline{\psi_+(k_1 k_2 k_3)} \psi_+(k'_1 k_2 k_3) + (+ \leftrightarrow -) \right\} \\ &= \sum_i \int dk_2 dk_3 \int_0^{\infty} dk_1 \frac{1}{k_1} b_i(k_1; k_2, k_3)^2 \{ |\psi_+|^2 + |\psi_-|^2 \} = 1, \end{aligned} \quad (72)$$

where $\psi_{\pm}(\mathbf{k}) \equiv \langle \mathbf{k}, \pm | \psi \rangle$. Since $|\psi\rangle$ can range through a dense set this yields

$$\sum_i \left(\frac{b_i(k_1; k_2, k_3)}{\sqrt{k_1}} \right)^2 = 1, \quad k_1 > 0. \quad (73)$$

For states $|\psi\rangle$ with $\psi_{\pm}(\mathbf{k})$ vanishing at $k_1 = 0$ one easily calculates that $\langle \psi | \hat{T} | \psi \rangle$ is independent of b_i and that for ΔT^2 the only b_i dependent term is of the form

$$\int dk_2 \int dk_3 \int_0^{\infty} dk_1 \frac{1}{k_1} \sum_i \left(\partial_1 \frac{b_i}{\sqrt{k_1}} \right)^2 \{ |\psi_+|^2 + |\psi_-|^2 \} \quad (74)$$

where again the reality of b_i is crucial. For ΔT^2 to be minimal this implies $\partial_1(b_i/\sqrt{k_1}) = 0$ or

$$\frac{1}{\sqrt{k_1}} b_i(k_1; k_2, k_3) = c_i(k_2, k_3). \quad (75)$$

From (73) it follows that

$$\sum_i (c_i(k_2, k_3))^2 = 1. \quad (76)$$

Inserting (75) into (70) and using (76) then gives

$$\begin{aligned} \hat{\Pi}_{f0}^A &= \frac{\hbar}{2\pi m} \int_{-\infty}^{\infty} dk_2 \int_{-\infty}^{\infty} dk_3 \int_0^{\infty} dk_1 \int_0^{\infty} dk'_1 \\ &\quad \sqrt{k_1 k'_1} \{ |\mathbf{k}, +\rangle \langle k'_1 k_2 k_3, +| + |\mathbf{k}, -\rangle \langle k'_1 k_2 k_3, -| \}. \end{aligned} \quad (77)$$

Inserting for $|\mathbf{k}, \pm\rangle$ from (66) one obtains the expression in (65) for $t = 0$. The operator $\hat{\Pi}_{f_t}^A$ is then obtained from (9). Since $\hat{\Pi}_{f_0}^A$ commutes with \hat{P}_2 and \hat{P}_3 , only \hat{P}_1^2 remains and this yields (65).

The absence of coherences between positive and negative k_1 components in (65) is due to the assumed reflection invariance. Recall that invariance under Galilei transformations as in [13] was not used here, only invariance under translations of the plane $x_1 = 0$ is assumed.

If instead of the plane $x_1 = 0$ one considers arrivals at the plane $x_1 = a$, the corresponding probability distribution operator is obtained by a spatial translation, which leads to an additional factor $\exp\{i(k_1 - k'_1)a\}$ in (65).

5. Interactions: conditional and operator-normalized arrival times

In the derivation of the general form of covariant time operators the normalization to 1 of the probability distribution is an essential condition. However, a free particle in two dimensions will arrive at a finite interval with a probability less than 1, and similarly in three dimensions. For a particle in a potential, also the arrival probability at a plane may be less than 1, due to scattering, and moreover, there may be several arrivals. Experimentally, in such a case one may measure the first time of arrival at a given position for a large number of replicas of the system and determine their distribution with respect to the total number of replicas. This distribution is, in general, not normalized to 1 since there may be systems with no arrival occurring. Dividing by the total probability for a first arrival or, equivalently, considering only those systems for which an arrival has actually been found, one obtains the conditional first-arrival probability distribution. Although this is, by construction, normalized to 1, it is not bilinear in the state vector and not the expectation of an operator. Alternatively, one may consider operator normalization as in [16, 17, 18] and then apply the techniques of Section 2. The physical relevance and interpretation of operator-normalized distribution in terms of a modification of the initial state has been pointed out in [18].

The operator for the (possibly non-normalized) distribution of first arrivals is again denoted by $\hat{\Pi}_t^A$ and the operator for the total probability for arrival at a given location by \hat{N} . One has

$$\hat{N} = \int_{-\infty}^{\infty} dt \hat{\Pi}_t^A. \quad (78)$$

For a given state $|\psi\rangle$ the conditional distribution, denoted by $\Pi_{ct}^{A\psi}$ for the times of first arrivals is the given by

$$\Pi_{ct}^{A\psi} = \frac{\langle\psi|\hat{\Pi}_t^A|\psi\rangle}{\langle\psi|\hat{N}|\psi\rangle}, \quad (79)$$

which is evidently not bilinear in $|\psi\rangle$. Since \hat{N} is a positive operator, $\hat{N}^{-1/2}$ exists on states on which \hat{N} does not vanish and which can be taken care of by a projector. If the external potential remains finite or is not too singular one expects from tunneling

that for any state there is a finite arrival probability, i.e. that $\hat{N}|\psi\rangle$ will never vanish. One can therefore define the operator $\hat{\Pi}_{Nt}^A$ by

$$\hat{\Pi}_{Nt}^A \equiv \hat{N}^{-1/2} \hat{\Pi}_t^A \hat{N}^{-1/2}. \quad (80)$$

Its time integral is then the unit operator and therefore the distributions determined by $\hat{\Pi}_{Nt}^A$ are normalized to 1. If \hat{N} and $\hat{\Pi}_{Nt}^A$ are known one obtains $\hat{\Pi}_t^A$ from (80).

To the normalized operator distribution $\hat{\Pi}_{Nt}^A$ one can apply the procedures of Section 2 if additional symmetries hold. Physically motivated symmetries of $\hat{\Pi}_t^A$ carry over to \hat{N} and thus also over to $\hat{\Pi}_{Nt}^A$. More tricky is the requirement of minimal variance under given symmetry conditions. Physically, one would require minimal variance for the conditional distribution, i.e. that $\hat{\Pi}_t^A$ is chosen in such a way that $\Pi_{ct}^{A\psi}$ has minimal variance for each $|\psi\rangle$ among all candidates satisfying the symmetry requirements. From (79) one has

$$\Pi_{ct}^{A\psi} = \left\langle \frac{\psi}{\|\hat{N}^{1/2}|\psi\rangle\|} \middle| \hat{\Pi}_t^A \middle| \frac{\psi}{\|\hat{N}^{1/2}|\psi\rangle\|} \right\rangle. \quad (81)$$

If one defines the normalized vector $|\psi_N\rangle$ by

$$|\psi_N\rangle \equiv \frac{\hat{N}^{1/2}|\psi\rangle}{\|\hat{N}^{1/2}|\psi\rangle\|} \quad (82)$$

one can write

$$\Pi_{ct}^{A\psi} = \langle \psi_N | \hat{N}^{-1/2} \hat{\Pi}_t^A \hat{N}^{-1/2} | \psi_N \rangle = \langle \psi_N | \hat{\Pi}_{Nt}^A | \psi_N \rangle. \quad (83)$$

For given \hat{N} , the correspondence between $|\psi\rangle$ and $|\psi_N\rangle$ is one to one and therefore, if $\hat{\Pi}_t^A$ leads to minimal variance the same is true for $\hat{\Pi}_{Nt}^A$, as long as \hat{N} is kept fixed. Therefore, one may look for a normalized operator distribution satisfying required symmetry conditions and minimal variance, as in Section 2. If in addition the operator \hat{N} for the total probability for arrival at a given location is known, one then obtains the physically interesting conditional probability distribution from Eqs. (80) and (79).

To exemplify this, we consider one-dimensional motion in a bounded potential. The latter is assumed to be invariant under space reflection about the origin, and we consider an ensemble of particles which originally came in from $\pm\infty$. For an ensemble of classical particles there are two types of individual trajectories. A particle coming in from $-\infty$ ($+\infty$) will either be reflected before it reaches the origin or, if it reaches the origin, will then continue to $+\infty$ ($-\infty$), by the symmetry of the potential. We consider first arrivals at the origin. The corresponding classical arrival time distribution has certain symmetries. Indeed, from the reflection invariance of the potential, in the ensemble obtained by space reflecting each trajectory of the original ensemble has the same distribution for arrivals at the origin as the original ensemble. Going over to the time reversed trajectories one concludes, as in Section 4 for the time reversed ensemble, that the arrival time distribution is obtained from the original one by replacing t by $-t$.

These symmetry properties are now carried over to the quantum case by demanding corresponding symmetries for $\hat{\Pi}_t^A$, i.e. invariance under space reflection and covariance

under time reversal. This implies the corresponding properties for the operator-normalized $\hat{\Pi}_{Nt}^A$ and in particular invariance of $\hat{\Pi}_{N0}^A$ under space reflection and time reversal. This then is the same situation as in Example 1 of Section 3 where a clock operator with the similar symmetry properties was constructed. Therefore, for $\hat{\Pi}_{N0}^A$ one obtains the same result as in (40), where, as a reminder, $|E, \pm\rangle$ denote eigenstates of \hat{H} such that $\langle x|E, \pm\rangle$ are real wavefunctions which are either symmetric or antisymmetric. From this expression and Eqs. (7) - (11) one then obtains $\hat{\Pi}_{Nt}^A$.

To determine the corresponding conditional probability distribution \hat{N} is needed, the operator for the total arrival probability at the origin. An at least approximate expression for \hat{N} may be obtained by modeling the detection process. The simplest way to do this is by a complex potential at the origin or by a fluorescence model (cf. [19] for a review of these models). From the \hat{N} calculated in this way and from the above result for $\hat{\Pi}_{Nt}^A$ one then obtains an expression for the conditional distribution of arrivals at the origin. The complex potential and fluorescence models also allows the calculation of an approximate expression for the conditional arrival distribution, and one may then compare the two expressions, in particular whether the abstractly obtained operator-normalized distribution together with the approximate result for \hat{N} leads to smaller variances than the distributions derived from the models.

This example can be carried over to three dimensions and a Hamiltonian of the form

$$\hat{H} = \hat{\mathbf{P}}^2/2m + V(|\hat{X}_1|), \quad (84)$$

using techniques similar to those described in Appendix A.3.

6. Discussion

We have derived the most general form of covariant time operators with a normalized probability distribution. The result has been applied to clock time operators and to time-of-arrival operators. To arrive at a unique operator, the multitude of possible operators has been restricted by physically motivated symmetry requirements, in particular time reversal invariance and, to obtain an optimally sharp observable, by the requirement of minimal variance.

Our general result has allowed us not only to weaken the assumptions of Kijowski [13] but at the same time generalize his arrival-time distribution for free particles arriving at a plane. It had been required in [13] that the distribution should be invariant under Galilei transformations which transform the plane into itself. As shown here, Galilei transformations are not needed and translation invariance is sufficient. Moreover, the restriction that the particles should come in from one side of the plane only has been lifted.

A free particle in three dimensions will arrive at a location of finite extent only with a probability less than 1, and also for a particle in a potential the arrival probability at a plane may be less than 1, due to scattering, and moreover, there may be several arrivals.

In an actual and repeated measurement one can consider only those outcomes for which at least one arrival has actually been found at some time and then in addition consider only the distribution of the times of the first arrival. This amounts to a division by the total arrival probability and determines the (normalized) conditional first-arrival probability distribution. However, the latter is not bilinear in the state vector, due to the division. As an alternative, we have applied operator normalization to the original distribution, and then one can apply the general results. The distribution thus obtained leads to the conditional distribution if the total arrival probability is known.

It should be pointed out that the probability distribution associated with an observable is in general of more direct experimental relevance than the operator of the observable itself because in most circumstances first the distribution of individual measurement results for a given state is obtained and then the expectation value is derived from that. For a particle in a potential, the total arrival probability at a plane may be less than one. In such a case there may still be a non-normalized temporal probability distribution operator but not necessarily an associated time operator. As has been pointed out above, the conditional probability distribution is in general not bilinear in the state vector and so cannot be used directly to construct a time operator.

In order to be meaningful, any experimental procedure purported to be the realization of a measurement of arrival times or of a quantum clock has to satisfy certain requirements, and the so constructed ideal observables provide guide-lines for these requirements. In this context, an analysis of this kind for the ideal arrival time-of-arrival distribution of [13] has been carried out in terms of an operational quantum-optical realization with cold atoms (cf. [19] for a review).

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Appendix A. Mathematical details

Appendix A.1. Nondegenerate energy spectrum

In this appendix, mathematical details are given to justify some more formal arguments in the main text. To illustrate the crucial points we first treat the case of a Hamiltonian \hat{H} with a simple absolutely continuous spectrum from $[E_0, \infty)$ or $(-\infty, \infty)$, with no degeneracy. The generalized eigenvectors can then be denoted by $|E\rangle$, with normalization $\langle E|E'\rangle = \delta(E - E')$. In the Hilbert space, \mathcal{H} , of the Hamiltonian we denote by $\mathcal{S}(\hat{H})$ and $\mathcal{D}(\hat{H})$ the subspaces of vectors $|\psi\rangle \in \mathcal{H}$ such that $\langle E|\psi\rangle \equiv \psi(E)$ is in the Schwartz space $\mathcal{S}(\mathbb{R})$ or $\mathcal{D}(\mathbb{R})$, respectively. Then $\hat{\Pi}_0 = -i[\hat{H}, \hat{F}_0]/\hbar$ from (4) is a positive semi-definite continuous sesquilinear form on $\mathcal{S}(\hat{H})$ or $\mathcal{D}(\hat{H})$ and, by

continuation, on $\mathcal{S}(\mathbb{R})$ or $\mathcal{D}(\mathbb{R})$. Hence, by the kernel theorem, it defines a distribution on $\mathcal{S}(\mathbb{R}^2)$ or $\mathcal{D}(\mathbb{R}^2)$, respectively, formally denoted by

$$\Pi_0(E, E') \equiv \langle E | \hat{\Pi}_0 | E' \rangle . \quad (\text{A.1})$$

Let $\left\{ |g_i\rangle \in \mathcal{D}(\hat{H}) , i = 1, \dots \right\}$ be maximal set (finite or infinite) such that

$$\langle g_i | \hat{\Pi}_0 | g_j \rangle = \delta_{ij} . \quad (\text{A.2})$$

We put $g_i(E) \equiv \langle E | g_i \rangle$ and define $b_i \in \mathcal{S}'(\mathbb{R})$ by

$$b_i(E) = \sqrt{2\pi\hbar} \int dE' \Pi_0(E, E') g_i(E') . \quad (\text{A.3})$$

Then

$$\langle g_\alpha | b_i \rangle \equiv \int dE \overline{g_\alpha(E)} b_i(E) = \sqrt{2\pi\hbar} \delta_{\alpha i} \quad (\text{A.4})$$

and, therefore,

$$\sum_i \langle g_\alpha | b_i \rangle \langle b_i | g_\beta \rangle = 2\pi\hbar \delta_{\alpha\beta} . \quad (\text{A.5})$$

With $\mathcal{L}\{g_i\}$ the linear span of the $g_i(E)$'s one therefore has, on $\mathcal{L}\{g_i\} \times \mathcal{L}\{g_i\}$,

$$\langle E | \hat{\Pi}_0 | E' \rangle = \frac{1}{2\pi\hbar} \sum_i b_i(E) \overline{b_i(E')} . \quad (\text{A.6})$$

If $\mathcal{N} \subset \mathcal{S}(\mathbb{R})$ or $\subset \mathcal{D}(\mathbb{R})$ defines the null space of (the distribution defined by) $\hat{\Pi}_0$, then $\mathcal{L}\{g_i\} \cup \mathcal{N}$ span $\mathcal{S}(\mathbb{R})$ or $\mathcal{D}(\mathbb{R})$, respectively, and therefore, by continuity, (A.6) holds also on $\mathcal{S}(\hat{H}) \times \mathcal{S}(\hat{H})$ and $\mathcal{D}(\hat{H}) \times \mathcal{D}(\hat{H})$, respectively.

Exploiting normalization. From Eqs. (5) and (A.6) one obtains, for a normalized $|\psi\rangle \in \mathcal{S}(\hat{H})$,

$$\begin{aligned} 1 &= \int \frac{dt}{2\pi\hbar} \langle \psi | e^{-i\hat{H}t/\hbar} \hat{\Pi}_0 e^{i\hat{H}t/\hbar} | \psi \rangle \\ &= \sum_i \int d\tau \left| \frac{1}{\sqrt{2\pi}} \int dE e^{iE\tau} \overline{b_i(E)} \psi(E) \right|^2 . \end{aligned} \quad (\text{A.7})$$

This implies that, for each i , the inner integral, considered as a function of τ , is square integrable, and so is its Fourier transform. The latter, as a distribution, is given by $\overline{b_i(E)} \psi(E)$ and hence is equivalent to a square integrable (i.e. L^2) function. Hence $b_i(E)$ is not only a distribution but even locally an L^2 -function. From (A.7) one then has by Parseval's theorem

$$\sum_i \int dE |b_i(E) \psi(E)|^2 = 1 . \quad (\text{A.8})$$

Since this is true for any normalized $|\psi\rangle \in \mathcal{S}(\hat{H})$, this implies

$$\sum_i \overline{b_i(E)} b_i(E) = 1 \quad \text{for almost all } E. \quad (\text{A.9})$$

Conversely, if a sequence of locally L^2 -functions satisfies (A.9), then $\hat{\Pi}_0$ defined by (A.6) gives rise to a covariant time operator through Eqs. (5) and (1).

Exploiting the second moment. We assume that for a dense set of $|\psi\rangle$ in $\mathcal{S}(\hat{H})$ the second moment exists, i.e.

$$\int \frac{dt}{2\pi\hbar} t^2 \langle \psi | e^{-i\hat{H}t/\hbar} \hat{\Pi}_0 e^{i\hat{H}t/\hbar} | \psi \rangle < \infty . \quad (\text{A.10})$$

With (A.6) this can be written as

$$\hbar^2 \sum_i \int d\tau \tau^2 \left| \frac{1}{\sqrt{2\pi}} \int dE e^{iE\tau} \overline{b_i(E)} \psi(E) \right|^2 . \quad (\text{A.11})$$

This implies that, for each i , the inner integral considered as a function of τ is not only square integrable but is also in the domain of the operator “multiplication by τ ”. Therefore, by standard results, the Fourier transform of this function, given by $\overline{b_i(E)}\psi(E)$, is not only in L^2 but is also absolutely continuous and has a derivative which is also in L^2 . Again by Parseval’s theorem one has

$$\text{second moment} = \hbar^2 \sum_i \int dE \left| \partial_E \left(\overline{b_i(E)} \psi(E) \right) \right|^2 < \infty . \quad (\text{A.12})$$

Since $|\psi\rangle$ is from the dense set $\mathcal{S}(\hat{H})$, b_i must also be absolutely continuous and its derivative exists almost everywhere and is locally L^2 . Using (A.9) one obtains

$$\text{second moment}/\hbar^2 = \quad (\text{A.13})$$

$$\int dE |\partial_E \psi|^2 + \int dE \sum_i |b'_i \psi|^2 + 2 \operatorname{Re} \int dE \sum_i \overline{b'_i} b_i \bar{\psi}' \psi \quad (\text{A.14})$$

In a similar way one finds

$$\langle \psi | \hat{T} | \psi \rangle = \int dE \bar{\psi} i\hbar \partial_E \psi + \int dE |\psi|^2 \sum b_i i\hbar \partial_E \overline{b_i} . \quad (\text{A.15})$$

We note that if the b_i ’s are real then (A.9) implies $\sum b_i(E) b'_i(E) = 0$ for almost all E and thus for real b_i ’s the last term in (A.14) as well as in (A.15) vanishes.

Appendix A.2. Extension to degenerate energy spectrum.

In case of a discrete degeneracy label we use the normalization as in (13) where for simplicity we assume the same degeneracy for each E . (The general case can be treated by direct integrals of Hilbert spaces). Then $\Pi(E, E')$, $g_i(E)$ and $b_i(E)$ from the nondegenerate case are replaced by $\Pi(E, \alpha, E', \alpha')$, $g_i(E, \alpha)$ and $b_i(E, \alpha)$, respectively, and (A.6) can be written as

$$\langle E, \alpha | \hat{\Pi}_0 | E', \alpha' \rangle = \frac{1}{2\pi\hbar} \sum_i b_i(E, \alpha) \overline{b_i(E', \alpha')} . \quad (\text{A.16})$$

By the same technique as above the normalization condition now implies

$$\sum_i b_i(E, \alpha) \overline{b_i(E, \alpha')} = \delta_{\alpha\alpha'} . \quad (\text{A.17})$$

Finiteness of the second moment implies that $b_i(E, \alpha)$ is absolutely continuous in E for each α and its derivative is locally L^2 .

In case of a continuous degeneracy label we use the normalization

$$\langle E, \lambda | E' \lambda' \rangle = \delta(E - E') \delta(\lambda - \lambda') \quad (\text{A.18})$$

This can be reduced to the discrete case by choosing a complete orthonormal set $\{\Phi_\alpha(\lambda), \alpha = 1, 2, \dots\}$ and putting

$$|E, \alpha\rangle \equiv \int d\lambda \Phi_\alpha(\lambda) |E, \lambda\rangle, \quad \alpha = 1, 2, \dots \quad (\text{A.19})$$

It can also be treated directly by replacing the functions $g_i(E)$ by $g_i(E, \lambda)$ and $b_i(E)$ by $b_i(E, \lambda)$. Then (A.17) is replaced by the equation

$$\sum_i b_i(E, \lambda) \overline{b_i(E, \lambda')} = \delta(\lambda - \lambda') \quad (\text{A.20})$$

valid for almost all E .

Appendix A.3. The case of partial translation invariance

To illustrate some mathematical details for Section 4 we consider for notational simplicity the two-dimensional case. We search for a covariant probability distribution operator, denoted by $\hat{\Pi}_t^A$, which is invariant under reflection $\sigma : \mathbf{x} \rightarrow -\mathbf{x}$, under translations which leave the line $x_1 = 0$ invariant, as well as under time reversal $\hat{\Theta}$, and which has minimal variance. Let \hat{H}_1 be the one dimensional Hamiltonian

$$\hat{H}_1 = \hat{P}_1^2 / 2m \quad (\text{A.21})$$

in the Hilbert space $\mathcal{H}_1 \equiv L^2(\mathbb{R})$ and denote by $|E_1, \pm\rangle$ the real symmetric resp. antisymmetric eigenstates of \hat{H}_1 , similarly as in Example 1 of Section 3. The eigenstates of \hat{H} are then

$$|E_1, \pm\rangle |k_2\rangle. \quad (\text{A.22})$$

The assumed invariances imply the corresponding invariances of $\hat{\Pi}_0^A$ and of \hat{F}_0^A . The expectation value of the latter gives the probability of finding a measured time value in $(-\infty, 0)$, and so $0 \leq \hat{F}_0^A \leq 1$. If $|\psi\rangle \in \mathcal{H}$, the formal expression

$$|\psi(k_2)\rangle \equiv \langle k_2 | \psi \rangle \quad (\text{A.23})$$

can be regarded, for each k_2 , as a vector in \mathcal{H}_1 , i.e. as a vector function of k_2 with values in \mathcal{H} , and for $|\psi_1\rangle, |\psi_2\rangle \in \mathcal{H}$ one has

$$\int dk_2 \langle \psi_1(k_2) | \psi_2(k_2) \rangle_{\mathcal{H}_1} = \langle \psi_1 | \psi_2 \rangle \quad (\text{A.24})$$

where the index indicates the scalar product in \mathcal{H}_1 . Each bounded operator \hat{A} which commutes with \hat{P}_2 satisfies

$$\langle k_2 | \hat{A} | k'_2 \rangle = \delta(k_2 - k'_2) \hat{A}(k_2), \quad (\text{A.25})$$

where $\hat{A}(k_2)$ acts in \mathcal{H}_1 , and thus

$$\langle k_2 | \hat{A} | \psi \rangle = \hat{A}(k_2) | \psi(k_2) \rangle . \quad (\text{A.26})$$

In a rigorous way this can be expressed in terms of direct integrals of Hilbert spaces,

$$\mathcal{H} = \int_{\oplus} dk_2 \mathcal{H}(k_2) , \quad \text{where } \mathcal{H}(k_2) \equiv \mathcal{H}_1 , \quad (\text{A.27})$$

with $|\psi\rangle$ corresponding to a vector-valued function $|\psi(\cdot)\rangle$, with $|\psi(k_2)\rangle \in \mathcal{H}(k_2)$, and \hat{A} corresponding to an operator-valued function $\hat{A}(\cdot)$ satisfying (A.26). If \hat{A} is positive and bounded by 1 then so is $\hat{A}(k_2)$, for almost all k_2 .

We now take \hat{F}_0^A for \hat{A} . Since \hat{H}_1 acts in each $\mathcal{H}(k_2)$, the action of $\hat{\Pi}_0^A$ is given by

$$\hat{\Pi}_0^A(k_2) \equiv \frac{-i}{\hbar} \left[H_1, \hat{F}_0^A(k_2) \right] \quad (\text{A.28})$$

considered as a bilinear form in each $\mathcal{H}(k_2)$. For almost all k_2 , $\hat{\Pi}_0^A(k_2)$ is a positive bilinear form satisfying invariance under $\hat{\sigma}$ and $\hat{\Theta}$. Hence each $\hat{\Pi}_0^A(k_2)$ is given by (40), (with E replaced by E_1). This finally implies

$$\hat{\Pi}_0^A = \frac{1}{2\pi\hbar} \int dE_1 dE'_1 \left\{ |E_1, +\rangle \langle E_1, +| + |E_1, -\rangle \langle E'_1, -| \right\} \quad (\text{A.29})$$

or, equivalently,

$$\begin{aligned} \langle \psi | \hat{\Pi}_0^A | \psi \rangle &= \frac{1}{2\pi\hbar} \int dk_2 dE_1 dE'_1 \\ &\quad \left\{ \langle \psi | E_1 + \rangle | k_2 \rangle \langle k_2 | \langle E'_1, + | \psi \rangle + \langle + \leftrightarrow - \rangle \right\}. \end{aligned} \quad (\text{A.30})$$

In three dimensions, the procedure is analogous. Now (77) results by a change of variable.

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